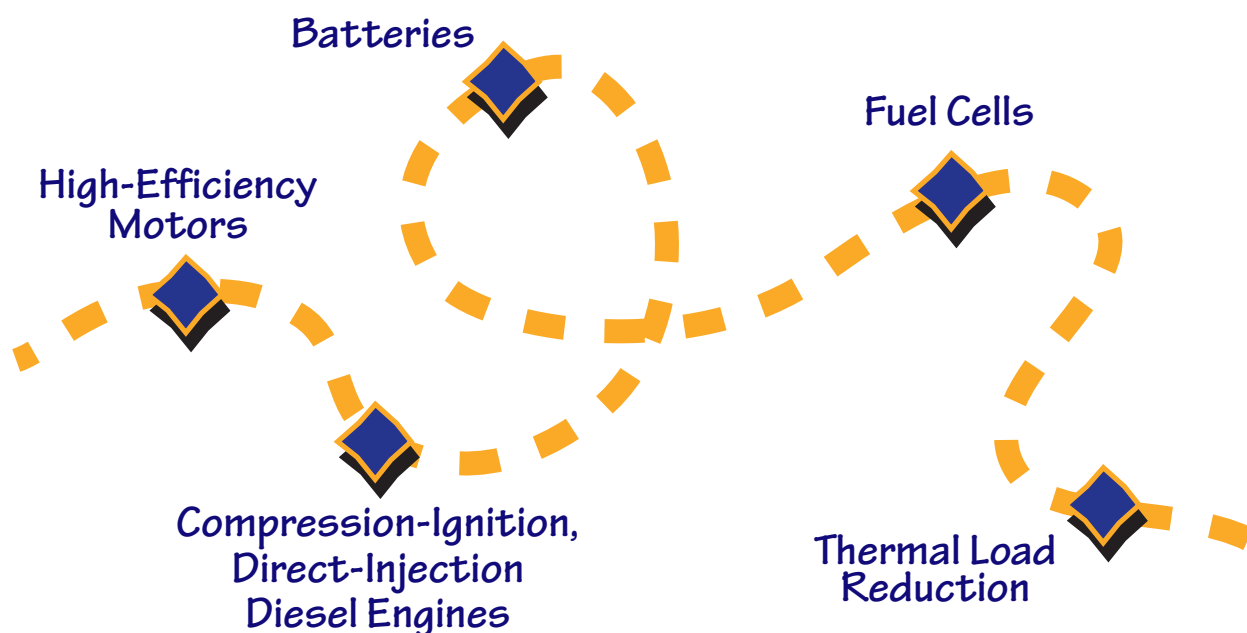




Cooperative Automotive Research for Advanced Technology

Snapshots of CARAT Projects, Phase 2



March 2000

Foreword

The U.S. Department of Energy's Cooperative Automotive Research for Advanced Technology (CARAT) program takes the most promising ideas for advanced, energy-efficient automotive technologies from small businesses and universities, funds their development from bench-scale models to engineering-scale prototypes, and then matches these concepts to manufacturers or suppliers with the know-how and resources to put them on the market. CARAT provides an expressway to validation for innovative technologies through a three-phase program of research and development.

In Phase 1, the objective is to prove the feasibility of advanced technologies by building bench-scale models, analyzing performance data, and identifying cost and manufacturing barriers. Phase 2 focuses on prototype development, while Phase 3 will culminate in technology validation. At the completion of each phase, the Department of Energy selects a few projects from the pool of program participants to continue on to the next hurdle, on the basis of technical feasibility, commercial potential, and available funding.

In the first round, 26 projects were funded for a period of one year, at about \$150,000 each. The researchers developed advanced concepts for fuel-efficient, low-emission automotive technologies in the areas of fuel cells, batteries, diesel engine emission reduction, vehicle system auxiliaries, and electric motors. In September 1999, at the CARAT Forum held in Troy, Michigan, results and data from Phase 1 of the CARAT program were presented to representatives from auto companies and subsystem/component suppliers. The response was very positive. Many attendees have developed relationships with the CARAT contractors that we hope will lead to commercialization of their technologies. The outcomes from these projects are posted on the CARAT website: www.ipd.anl.gov/carat.

The CARAT projects featured in this booklet were chosen from among the 26 Phase 1 projects selected to continue into Phase 2. Each is summarized by its principal investigator in a success story that includes a project overview, discussion of Phase 1 results, and description of future plans. These projects represent the most promising concepts – both technically and commercially – for enabling the realization of the future's energy-efficient automobiles.

Donna Lee Ho
CARAT Program Manager
Office of Advanced Automotive Technologies
Office of Transportation Technologies
Energy Efficiency & Renewable Energy
U.S. Department of Energy

New Higher-Performance, Low-Cost Coatings for Selective Solar Radiation Control

Energy Conversion Devices, Inc.

Project Overview

Air-conditioning, the single greatest auxiliary power load for cars, accounts for up to 15% of fuel consumption by conventional vehicles (50% in vehicles with very high fuel economy). Cars absorb heat mainly via solar radiation through the windows. This heat load is most effectively reduced by selective solar radiation control (SSRC) window coatings that transmit visible light, absorb ultraviolet radiation, and reflect the infrared (heat) portion of the spectrum. SSRC coatings are standard in architectural applications, but their use in cars is limited because of their cost, currently several dollars per square foot.

SSRC coatings, which have a thickness of only about one-third of a wavelength of visible light, typically comprise three relatively thick dielectric layers surrounding two thin layers of silver. Today, these coatings are made exclusively with magnetron sputtering technology. The need to deposit thick dielectric layers, which go on slowly, accounts for a major share of their cost. The key to reducing this cost, then, is a technology that can deposit dielectric layers quickly and cheaply.

At Energy Conversion Devices, Inc. (ECD), our development of the Microwave Plasma Enhanced Chemical Vapor Deposition (MPECVD) process has led to order-of-magnitude improvements in deposition rate and capital, material, power, and operating costs, compared with sputtering, for certain optical coating applications. In this work, we are collaborating with Southwall Technologies, Inc. (STI), a third-tier automotive supplier and the world's leading producer of high-performance automotive SSRC coatings.

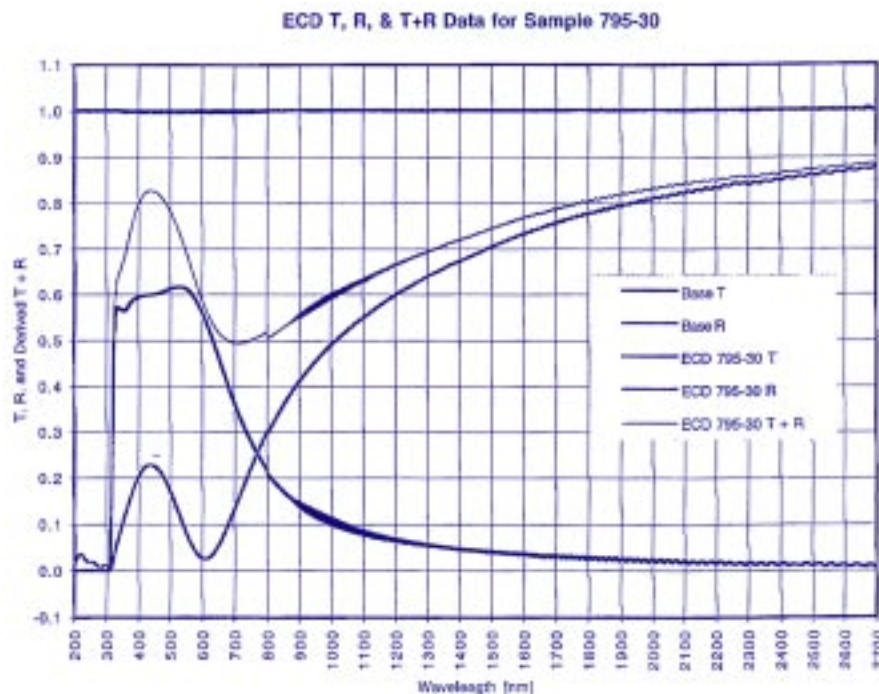


Figure 1. Reflection (R) and transmission (T) spectra as a function of wavelength for a prototype SSRC coating. The five-layer coating was produced by using ECD's MPECVD technology to deposit the thick (silicon dioxide, or quartz) layers and conventional DC sputtering to deposit the thin (silver) layers.

Phase 1 Results

Working with STI, we have demonstrated the technical and economic feasibility of applying our MPECVD technology to fabricate low-cost, high-performance SSRC coatings on a thin, flexible PET (polyester) substrate. Such coatings can be bonded between two layers of glass for automotive window applications. Our accomplishments in Phase 1 include the following:

- We performed optical modeling studies to design SSRC coatings based on MPECVD-deposited dielectric layers.
- We installed an STI sputtering cathode in ECD's pilot MPECVD deposition machine, which deposits dielectric layers onto 0.3-m-wide, 750-m-long, 2-mil-thick rolls of PET substrate.
- Using the pilot machine, we demonstrated simultaneous sputtering of thin silver layers and MPECVD deposition of thick dielectric layers in a single pass. The MPECVD process did not "burn off" the silver layers, as is common with sputtering systems, and we found that high-quality silver/dielectric coatings could be produced without the need for intermediate layers to protect the silver.
- We successfully produced both single-silver-layer (heat mirror) and double-silver-layer (SSRC) prototype coatings in our pilot machine, using the MPECVD process with a high deposition rate. Transmission and reflection spectra for one such coating produced are shown in Figure 1.
- We showed that material costs for this process would be approximately \$0.10/ft² (\$1.00/m²), substantially lower than for the sputtering process. Preliminary estimates indicate that the capital equipment cost for our machine will also be substantially lower because of our process's high deposition rate.

Future Plans

ECD's overall goal for Phase 2 is to optimize the new, low-cost MPECVD process and qualify the technology for producing SSRC coatings that meet or exceed present-day standards for mechanical, electrical, and optical performance, as well as durability. At the same time, we expect to be able to cut costs in half, or even less. To achieve this overall program goal, we have identified four principal areas of work: economic analysis and business planning, process development, product development, and system development (optimization for economy and throughput).

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Low-Cost Gas Sensors for Fuel-Cell-Powered Vehicles

Illinois Institute of Technology

Project Overview

In anticipating the widespread use of fuel-cell-powered vehicles, we presuppose certain technologies and components that are not available today. Such vehicles will generate and use flammable or potentially harmful gases, so sensors are needed that are highly selective for their target gases, as well as capable of meeting ordinary automotive standards (low cost, wide environmental range, and long lifetime). We are investigating basic gas sensor designs for lower cost and higher reliability: first for carbon monoxide (CO) and hydrogen, and later for hydrogen sulfide (H_2S) and other gases and vapors. Figure 1 shows the uses of gas sensors on a fuel cell vehicle; both process control and human health and safety applications are indicated.

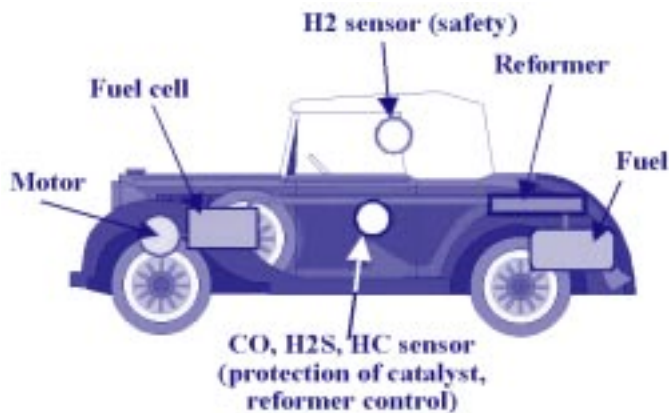


Figure 1. Gas sensors used on a fuel-cell vehicle.

The research will proceed in stages, developing

- A hydrogen sensor to measure leakage of this explosive gas into the passenger space over a range of 0.1-5% by volume in air, and
- A sensor to measure CO at 10 ppm, against a background of 40% hydrogen by volume, in reformat gas (CO control is needed to prevent poisoning of the fuel cell catalyst).

Later stages will include sensors for other fuel cell applications and analytes.

Although electrochemical sensors for hydrogen and CO have been available for decades, some specifications for automotive use have not yet been met. The technical challenges demand a dramatic rethinking of the design of conventional amperometric gas sensors to incorporate new catalysts, materials, and physical designs. An innovative approach is needed to produce a sensor that has the required sensitivity and selectivity, can remain operational for 10 years at elevated temperatures, and sells for about five dollars.

Phase 1 Results

- *Low-Cost Sensor Design.* We have taken part in developing a new physical design for a basic sensor topology that requires fewer parts and less catalyst. The new device is assembled in fewer steps and is ideally suited to mass production. The key difference in this design is its use of electrically conductive polypropylene to connect the internal active elements with exterior circuits, thereby reducing the parts count and all but eliminating electrolyte leaks, the most common cause of failure. Sensors based on this design are already in use in safety equipment. We have also developed a permeable membrane modification that has led to a high-range sensor for automotive tuning.
- *Hydrogen Sensor.* The hydrogen sensor poses two major problems. First, the platinum (Pt) electrode sensor responds to a large number of interferences. Since 1% hydrogen is 10,000 ppm, well above the expected concentrations of most interferences, the sensitivity of the sensor can be lowered by using a much-reduced access port and a thin permeable membrane. Second, and more serious, the sensor loses its sensitivity when exposed to high hydrogen concentrations because the gas penetrates to the reference electrode. The reference electrode can be relocated in the sensor, and alternative reference electrodes can be used that are not sensitive to hydrogen. We can also employ permeable polymer membranes to reduce the sensitivity and ensure linearity over the required range. We have taken preliminary steps toward carrying out these modifications, with encouraging initial results.

- *Carbon Monoxide Sensor*: Making a sensor that responds to less than 100 ppm CO yet rejects hydrogen at 400,000 ppm has proven challenging. A traditional platinum-catalyzed CO sensor has a sensitivity to hydrogen that is 50-100 times less than the CO signal, and improvement by more than an order of magnitude has been achieved with a palladium catalyst. The hydrogen drift problem has been solved in the CO sensor, as illustrated in Figure 2; the reference electrode has been replaced to eliminate drift.

We are evaluating new catalysts and voltammetric procedures to bring about the dramatic increase in selectivity required.

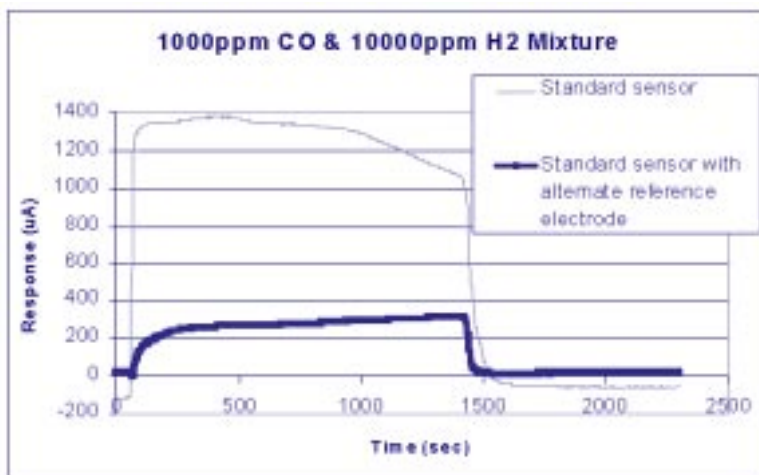


Figure 2. Elimination of hydrogen drift in the carbon monoxide sensor.

Future Plans

Continued examination of low-cost sensor designs is a priority. Fabrication of the working prototypes and evaluation of their performance will boost the automotive industry's confidence in this approach. We continue to improve the integrity of the bond between conductive plastic and metal electrodes, for example. The basic low-cost platform, which is very flexible, will be adapted to other sensors, such as for hydrogen sulfide and nitrogen oxides (NO_x).

On the basis of our Phase 1 findings, we will construct hydrogen sensors. A reference electrode that does not respond to hydrogen will be incorporated into the structure. Significant changes to the basic low-cost design will be required to mechanically move the reference electrode away from the porous membrane.

Work will continue on the CO process sensor. Additional requirements have been added, including operation at temperatures of 80°C or higher. This will mean incorporating new electrolytes, similar to those used in the fuel cell itself, into the sensor structure. The use of novel catalysts will continue to advance us toward our selectivity goals. We will investigate new sensors for such analytes as H_2S and NO_x .

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Comprehensive Computer Models for Simulating PEM Fuel Cell Performance

University of Miami

Project Overview

The University of Miami has developed two- and three-dimensional computer models that use a unified approach for proton-exchange-membrane (PEM) fuel cells. These models can be applied to different fuel cell elements; special forms for each element take into account different properties and processes. Using this approach, we solve the same set of equations in a unified domain with different properties, eliminating the need for arbitrary boundary conditions at various interfaces. Because inputs for the model match those in real-life fuel cell operations, we avoid errors from arbitrary or simplified boundary conditions.

We use object-design and object programming technology to link our models to a user-friendly interface. The control unit of the program is not coupled to the numerical modules, so improvements and new models can easily be incorporated. The package is easy to use, maintain, and update, and it readily adopts new technology.

Phase 1 Results

We have obtained very good simulation results with the preliminary models and software package we developed. Some of these results have been verified by fuel cell developers, as well as through comparison with experimental results from the literature.

Figure 1 shows a sample oxygen concentration distribution across the flow channel, the gas diffusion layer (GDL), and the catalyst layer. Earlier fuel cell models prescribed boundary conditions at the interface between the channel and the GDL. As can be seen, the oxygen concentration at this interface changes with current density and location along the channel. Our unified approach eliminates the errors introduced by simplified boundary conditions.

In Figure 2, we see the current-density distribution along the flow direction (x-coordinate) and across the channel (z-coordinate). Along the flow direction, the reactant concentration and the current density are higher at the inlet; across the channel, the current density is lower at the middle because of the blocking effect of the collector plate – most other models fail to include this effect.

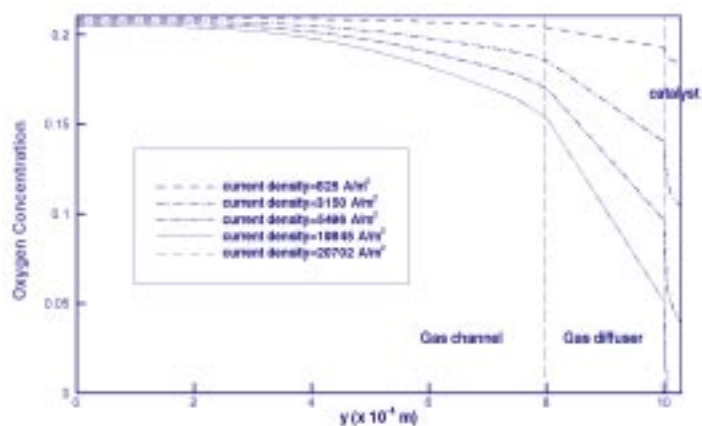


Figure 1. Oxygen concentration distribution in the cathode gas channel, gas diffuser, and catalyst layer.

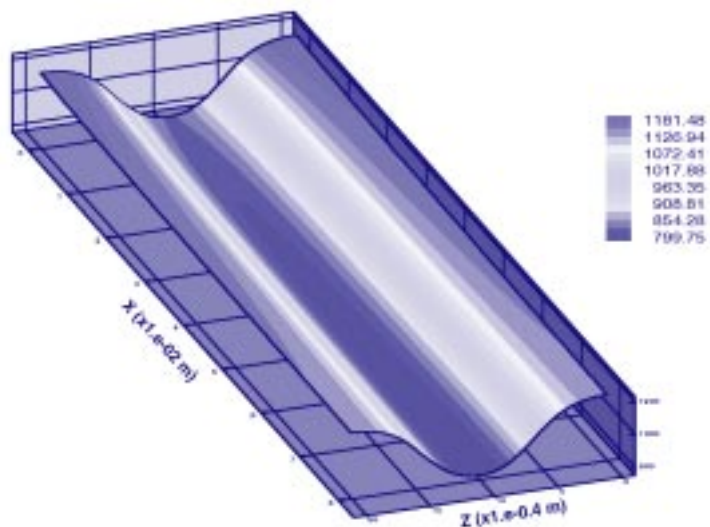


Figure 2. Current distribution from the three-dimensional model.

Figure 3 shows a sample temperature distribution across the entire fuel cell sandwich: two flow channels, two GDLs, two catalyst layers, and the membrane. Here, the cathode catalyst layer, where most of the heat is generated, has the highest temperature.

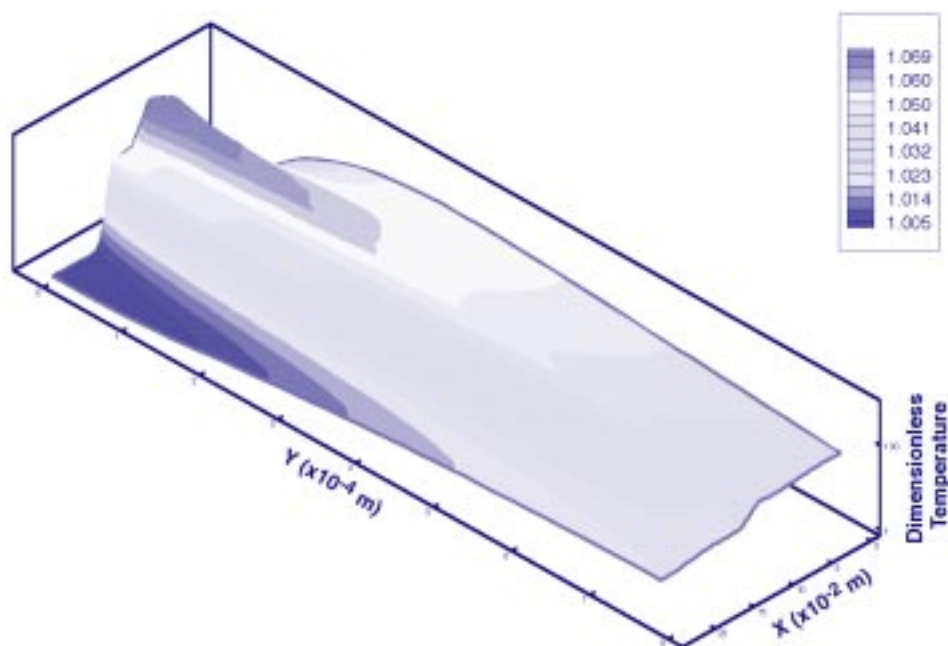


Figure 3. Temperature distribution across the fuel cell sandwich. From front to back: anode channel, gas diffuser, catalyst layer, membrane, catalyst layer, gas diffuser, and cathode channel (results are presented not according to physical scale, but rather to grids).

Future Plans

In Phase 2, the preliminary models we developed at the cell level for Phase 1 will be improved and extended to include a much wider range of operating conditions, such as using reformat on the anode side. In future efforts, models at the stack and system levels can also be developed.

The package will be stand-alone, with no other software required, so it will be both fast and cost-effective. Its flexibility will allow users to implement their own models to incorporate special applications and requirements. The friendly user interface will make this software accessible to any engineer or technician.

We will produce a comprehensive software package for the simulation, design, and optimization of fuel cells. The package will include one-, two-, and three-dimensional models, both steady-state and transient. Users can choose appropriate models for specific applications and accuracy requirements.

This project has been selected for CARAT Phase 2 funding. We have received numerous inquiries from companies working on fuel cells and related systems, and we are currently exploring ways to collaborate with several of them.

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Transition-Metal Carbide Water-Gas-Shift Catalysts

University of Michigan

Project Overview

Fuel cells are being developed to support the commercialization of cleaner, more fuel-efficient vehicles. In developing fuel cell vehicles, many manufacturers favor proton-exchange-membrane (PEM) cells designed to operate with hydrogen-rich feeds from hydrocarbon steam reforming or partial oxidation. Because PEM electrocatalysts can tolerate only small concentrations of carbon monoxide (CO), the water-gas-shift (WGS) reaction is a critical step during processing of the fuel cell feed. The WGS reactor typically constitutes about one-third of the mass, volume, and cost of the fuel processor. Although currently available catalysts work well in industrial petroleum refining and chemical plants, significantly improved catalysts are required to meet the transient operation and size constraints imposed by vehicular applications. Rather than seek incremental improvements by modifying existing formulations, we have demonstrated new WGS catalysts based on high-surface-area transition-metal carbides. The high activities, durabilities, and sulfur tolerance associated with these catalysts should result in significant reductions in WGS reactor size and cost.

Phase 1 Results

Our principal goal in Phase 1 was to validate carbide-based catalysts by demonstrating their high activities and durabilities for the WGS reaction. In bench-scale tests using unoptimized powders, several high-surface-area carbide catalysts equaled or surpassed commercial high-shift (iron-chromium, Fe-Cr) and low-shift (copper-zinc-aluminum, Cu-Zn-Al) catalysts in terms of activity. Figure 1 compares the rates for two of the carbide catalysts with those for the Cu-Zn-Al catalyst. Besides having high activities, the carbide catalysts were not deactivated during extended use or in tests where the materials were periodically exposed to condensate; in contrast, the commercial shift catalysts were deactivated during thermal cycling experiments. We also compared the properties of the carbide-based catalysts with those of a noble-metal-based catalyst; in this case, steady-state activities for the carbides exceeded those for a palladium/cerium oxide (Pd/ceria) catalyst.

Commercialization of carbide-based catalysts will require competitive production costs. By analogy with the production of high-surface-area molybdenum, we predict that the carbide catalysts will cost ~\$8/lb, compared with ~\$7/lb for commercial low-temperature shift catalysts. Taking into account their higher activities and durabilities and their tolerance to sulfur, we believe carbide-based WGS catalysts are sufficiently promising to warrant further development.

Future Plans

Vehicular vibrations and specified weight and volume targets are expected to require the use of monolithic substrates. In Phase 2, our principal goal is to demonstrate monolith-supported carbide catalysts that can be used in commercial fuel-cell-powered vehicles. Specific Phase 2 objectives are to

- Prepare highly active, sulfur-tolerant monolith-supported catalysts,
- Demonstrate improved performance in a prototype fuel processor, and
- Confirm the cost-competitiveness of these catalysts.

This work will be accomplished in collaboration with Catalite LLC; Nanodyne, Inc.; and United Catalysts, Inc. These partners were selected for their expertise in key areas involving commercialization of fuel processor catalysts. During Phase 3, we will work with fuel cell system and vehicle developers to fully evaluate fuel processors on the basis of carbide-based WGS catalysts.

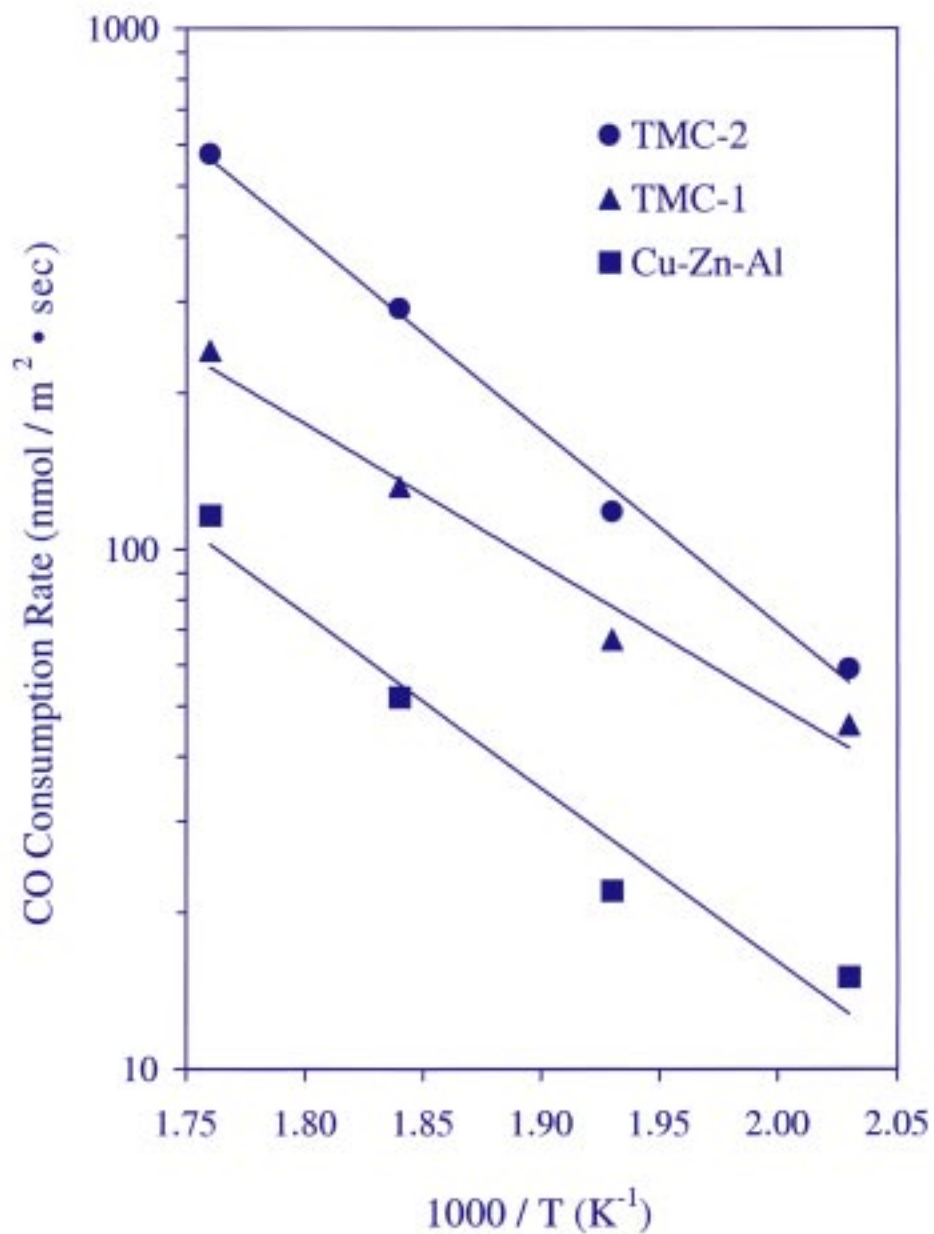


Figure 1. Carbon monoxide consumption rates for two transition-metal carbide (TMC) catalysts are compared with those of a commercial low-temperature shift catalyst (Cu-Zn-Al).

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Nanoscale Water-Gas-Shift Catalysts

NexTech Materials, Inc.

Project Overview

NexTech Materials is collaborating with the University of Pennsylvania, United Catalysts, Epyx, and International Fuel Cells to develop a new catalyst material. One goal of the Cooperative Automotive Research for Advanced Technology (CARAT) program is to develop superior water-gas-shift (WGS) catalysts for use in fuel processors that convert gasoline into a hydrogen-rich gas for automotive proton-exchange-membrane (PEM) fuel cells. The need for a fuel-processing system that is light and small enough to fit within the confined space of a vehicle – and can also perform reliably under highly variable power loads, provide rapid start-up, and deliver a gas stream with very low levels of carbon monoxide (CO) – presents a major technical hurdle. The WGS reactor, a critical component of the fuel processor, reduces the CO concentration to intermediate levels, which can then be further reduced in a subsequent preferential oxidation step. Commercial catalysts used for WGS reactions are unsuitable for transportation because of their insufficient reactivity (high weight and volume) and their tendency to degrade under the severe conditions encountered in an automotive system.

Our new catalyst material is based on nanoscale mixtures of cerium oxide (ceria) and uniformly incorporated platinum (Pt). We use advanced synthesis methods to prepare dispersed suspensions of nanoscale particles of cerium oxide, together with wet-chemical methods to deposit platinum onto the ceria nanoparticle surfaces.

Phase 1 Results

In Phase 1, we established the viability of Pt/ceria WGS catalysts:

- We evaluated a range of synthesis conditions for preparing Pt/ceria catalysts. Screening tests at the University of Pennsylvania (Figure 1) confirmed that Pt/ceria catalysts exhibited WGS rates that were slightly higher than those of commercial copper-based catalysts.
- Application-specific testing at United Catalysts confirmed that our Pt/ceria catalysts provide high performance and maintain stability at temperatures higher than 500°F.
- By means of cost/weight/volume modeling of WGS reactors based on ceramic monoliths washcoated with Pt/ceria catalysts (Table 1), we confirmed that the Partnership for a New Generation of Vehicles (PNGV) cost target (\$150) will be met with reactors having volumes of less than 6 L and weighing under 3 kg.

Table 1. Comparison of Washcoated Pt/Ceria Catalytic Monoliths with State-of-the-Art WGS Reactors (for a 50-kW fuel processor)

Criterion	Pt/Ceria	State of the Art
Cost (\$)	<150	300-500
Weight (kg)	< 3	20-40
Volume (L)	5-6	20-40
CO content (%)	0.3-0.6	<0.50

Future Plans

In Phase 2, NexTech's primary goals are to optimize the performance of ceria-based catalysts for both low- and high-temperature-shift reactors and to develop monolithic support technology for these catalysts. Phase 2 will culminate in a demonstration of monolith-supported catalysts in full-scale (50-kW) WGS reactors used in automotive fuel processors.

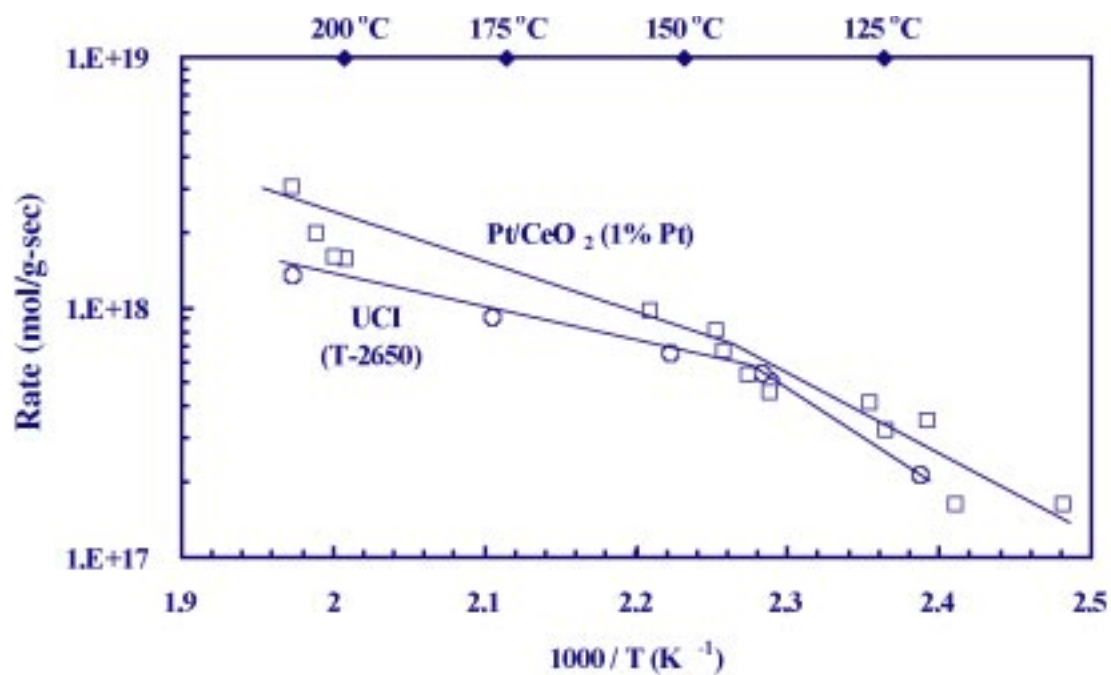


Figure 1. Arrhenius plots of WGS rates for a Pt/ceria catalyst and a precommercial copper-based catalyst (T-2650) being developed by United Catalysts.

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High-Temperature, Direct-Methanol-Fueled Proton-Exchange-Membrane Fuel Cells

Pennsylvania State University

Project Overview

Penn State University has commenced an interdisciplinary effort that brings together expertise in the design and synthesis of polyphosphazene polymer membranes with experience in the field of electrochemical engineering. Our goal is to develop a polymer electrolyte (proton-conducting) membrane capable of operating at elevated temperatures. High-temperature proton-exchange-membrane fuel cells (PEFCs) offer the following advantages:

- Faster reaction rates may lessen or even eliminate the need for noble metal catalysts and may lead to greater tolerance of carbon monoxide (CO) poisoning at the anode.
- Higher proton mobilities will be attained, reducing membrane resistivity.
- Higher temperatures will enhance the prospects for developing direct-fueled fuel cells (i.e., cells for which the fuel need not be reformed to hydrogen).

Phase 1 Results

We have synthesized and evaluated a new class of ion-exchange membranes for PEFCs. The membranes consist of polymers based on the polyphosphazene system, particularly those that contain sulfonate, carboxylate, phosphate, and phosphonate anion substituents. These polymers are used because of the thermo-oxidative and reductive stability of their phosphorus-nitrogen backbone and because they permit changes to be made in side-group structures to optimize membrane properties.

We have designed and built experimental systems to measure the electrochemical properties and methanol crossover of polyphosphazene membranes at elevated temperatures. In addition, we have developed an original fuel cell system for experimental measurements at temperatures up to 200°C.

Our most important achievement is the development of proton-conducting membranes, based on polyphosphazene polymers, that have much smaller methanol crossover than that of Nafion 117. At the same time, our polyphosphazene polymers and Nafion 117 display similar conductivities.

Future Plans

Future project plans include

- Further development of polyphosphazene polymers as fuel cell membranes.
- Development of new, proton-conducting individual cell assemblies for operation in direct-methanol fuel cells at elevated temperature (<200°C).
- Further development and optimization of a high-temperature, direct-methanol fuel cell system for experimental measurements at temperatures up to 200°C.

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Integrated AC Induction Motor/Inverter/ Cooling System for Light-Duty Electric Vehicle Drivetrains

YPT, Inc.

Project Overview

Our objective is to improve electric and hybrid electric vehicle traction systems – specifically, to develop a highly efficient, lower-cost motor controller system for high-volume automotive use.

The power density improvements and cost reductions sought by the Partnership for a New Generation of Vehicles (PNGV) for high-volume motors can be achieved only through increased motor speed. The power achievable from a given design is the product of speed and volume. Traction drives that use induction motors at speeds up to 12,000 rpm are common, but their use for traction at speeds above 15,000 rpm has not been explored. To meet CARAT program goals, we must raise the motor speed to 20,000 rpm, without sacrificing efficiency or durability.

Significant reductions in a traction system's size and weight lead to increased power density, but they also require a more comprehensive thermal management design. The power section of the inverter (contained within the motor housing) communicates with the control electronics (located in the passenger compartment) via fiber-optic cables. Integrating the inverter power section and the motor will significantly reduce radiated electromagnetic interference. (The integrated package will include the gearing needed to couple the motor to the vehicle drive system.)

Phase 1 Results

Our induction motor, designed around an industry-standard frame size, is fully compatible with existing motor manufacturing facilities. We derived complete loss maps and efficiency maps for the motor up to 21,000 rpm. We found that stray load losses were unacceptably high in the upper speed regions, but we improved efficiency at speeds above 15,000 rpm by modifying the designs. A dynamic analysis of the new motor design showed that the first critical speed was well above 20,000 rpm.

Firm price quotations cannot be obtained until all motor design details are completed, but we have estimated a moderate-volume price of about \$200 per unit from an induction motor manufacturer. If the system produces 100-kW power at the rated bus voltage, then the motor cost is approximately \$2/kW. Combining this with the cost of the gear reducer and housing, we expect the cost of the assembly to meet the PNGV goal of \$4/kW.

Team members designed a preliminary single-stage planetary gear reducer and developed a preliminary packaging concept for the integrated motor-inverter power unit and the vehicle control computer. A plan was also completed for developing a manufacturing process that will use low-temperature solders to mount standard insulated gate bipolar transistor-diode half-bridge modules to the heat sink. Improving the thermal impedance between the modules and the sink will help reduce the cost of the inverter power semiconductors.

Virginia Tech's mechanical engineering department developed thermal models for the inverter and the motor, as well as a solution algorithm for evaluating motor-inverter temperatures over specific duty cycles. The model's accuracy was confirmed by modeling an 80-frame design and comparing the results with laboratory data.

The loss maps derived for the motor and inverter can be used to drive both transient and steady-state thermal analysis for any duty cycle. Using these data, we have optimized the motor design in the low-torque region.

Future Plans

In Phase 2, the new induction motors will be built in a standard induction motor manufacturing facility. One motor, mounted in a conventional housing, will be used to confirm the basic design parameters. A second motor will be spun at increasing speeds to confirm the critical speed calculation. The remaining motors will be used in integrated power units. Single-stage planetary gear reducers, suitable for input velocities of 20,000 rpm, will be built and integrated into the power package. The package design will incorporate a common thermal management system for the motor and inverter. A new vehicle control computer will be designed, along with the fiber-optic communication system that links the computer and the power unit.

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